

WHAT IS CLAIMED IS:

1. A method, comprising steps of:

SUB A2 (A) synthesizing a first population of entities and detecting a property of each of said entities by a high throughput screening (HTS) method and

5 (B) executing a genetic algorithm based on said property of said entities to identify a second population of entities.

2. The method of claim 1, wherein said step (B) comprises at least one operation selected from (i) mutation, (ii) crossover, (III) mutation and selection (iv) crossover and selection and (v) mutation, crossover and selection.

10 SUB A3 3. The method of claim 1, comprising randomly identifying said first population of entities prior to synthesizing said first population according to step (A).

4. The method of claim 1, further comprising generating a binary string representing said first population of entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string
15 representing said second population of entities.

5. The method of claim 1, further comprising generating a binary string representing variable parameters of said first population of entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

20 6. The method of claim 1, further comprising generating a binary string representing variable parameters of entities, synthesizing said entities and selecting said first population from said entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string
SUB A4 representing said second population of entities.

25 7. The method of claim 1, further comprising generating a binary string representing variable parameters of entities, synthesizing said entities, evaluating said synthesized entities for a desired property, weighting said entities according to an

hierarchy of fitness of said property and selecting said first population as a sampling from said weighed entities and step (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

5 8. The method of claim 1, further comprising generating a binary string representing variable parameters of entities, synthesizing said entities, evaluating said synthesized entities for a desired property, pairing said entities and (B) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

10 9. The method of claim 1, further comprising generating a binary string representing variable parameters of entities, synthesizing said entities, evaluating said synthesized entities for a desired property and pairing said entities and (B) comprises executing a genetic algorithm comprising a uniform random crossover operator to produce a binary string representing said second population of entities.

15 10. The method of claim 1, further comprising generating a binary string representing variable parameters of entities, synthesizing said entities, evaluating said synthesized entities for a desired property, weighting said entities according to an hierarchy of fitness according to said property, selecting said first population as a sampling from said weighed entities and pairing said entities and step (B) comprises
20 executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

11. The method of claim 1, further comprising conducting steps (A) and (B) on said second population of entities to produce a third population of entities.

25 12. The method of claim 1, further comprising repeating steps (A) and (B) on said second population of entities and subsequent populations of entities until a fit entity is identified.

13. The method of claim 1, wherein said first population of entities is synthesized by steps of:

providing a first reactant system at least partially embodied in a liquid; and

contacting the liquid with a second reactant system at least partially embodied in a gas, the second reactant system having a mass transport rate into the liquid wherein the liquid forms a film having a thickness sufficient to allow a reaction rate that is essentially independent of the mass transport rate of the second reactant system into the liquid to synthesize said first population of entities.

14 The method of claim 1, further comprising synthesizing said second population of entities by steps of:

providing a first reactant system at least partially embodied in a liquid; and

contacting the liquid with a second reactant system at least partially embodied in a gas, the second reactant system having a mass transport rate into the liquid wherein the liquid forms a film having a thickness sufficient to allow a reaction rate that is essentially independent of the mass transport rate of the second reactant system into the liquid to synthesize said second population of entities.

15. The method of claim 1, wherein said HTS method is a combinatorial organic synthesis (COS).

16. The method of claim 1, wherein said first population of entities is a catalyst system.

17. The method of claim 1, wherein said first population of entities is a catalyst system comprising a Group VIII B metal.

18. The method of claim 1, wherein said first population of entities is a catalyst system comprising palladium.

19. The method of claim 1, wherein said first population of entities is a catalyst system comprising a halide composition.

20. The method of claim 1, wherein said first population of entities is a catalyst system that includes an inorganic co-catalyst.

21. The method of claim 1, wherein said first population of entities is a catalyst system that includes a combination of inorganic co-catalysts.

22. A high throughput screening (HTS) method, comprising:

5 (A) depositing each of a first population of entities in respective wells of an array;

(B) reacting said population to form a plurality of products;

(C) detecting a property of each of said plurality of products; and

(D) executing a genetic algorithm based on said property of said plurality of products to identify a second population of entities.

10 23. The method of claim 22, further comprising:

(E) depositing each of said second population of entities in respective wells of an array; and

(F) reacting said second population to form a second plurality of products.

15 24. The method of claim 22, comprising randomly identifying said first population of entities prior to depositing said first population according to step (A).

25. The method of claim 22, wherein said step (D) comprises an at least one operation selected from (i) mutation, (ii) crossover, (iii) mutation and selection (iv) crossover and selection and (v) mutation, crossover and selection.

20 26. The method of claim 22, further comprising generating a binary string representing said first population of entities and step (D) comprises executing a genetic algorithm with a processor on said binary string to produce a binary string representing said second population of entities.

27. The method of claim 22, wherein said HTS method is a combinatorial organic synthesis (COS).

28. The method of claim 22, wherein said first population of entities is a catalyst system.

29. The method of claim 22, wherein said first population of entities is a catalyst system comprising a Group VIII B metal.

5 30. The method of claim 22, wherein said first population of entities is a catalyst system comprising palladium.

31. The method of claim 22, wherein said first population of entities is a catalyst system comprising a halide composition.

10 32. The method of claim 22, wherein said first population of entities is a catalyst system that includes an inorganic co-catalyst.

33. The method of claim 22, wherein said first population of entities is a catalyst system that includes a combination of inorganic co-catalysts.

15 34. A method for preparing a diaryl carbonate which comprises contacting at least one hydroxyaromatic compound with oxygen and carbon monoxide in the presence of an amount effective for carbonylation of at least one catalyst composition comprising a Group VIIIB metal or a compound thereof, a bromide source and a polyaniline wherein said catalyst composition is selected according to a genetic algorithm screening process.

20 35. The method of claim 34, wherein at one of said Group VIIIB metal or compound thereof, said bromide source and said polyaniline is selected by said genetic algorithm screening process.

36. The method of claim 34, wherein a concentration of at least one of said Group VIIIB metal or compound thereof, said bromide source and said polyaniline is selected by said genetic algorithm screening process.

25 37. The method of claim 34, wherein said Group VIIIB metal or compound thereof, said bromide source and said polyaniline are selected by said genetic algorithm screening process.

38. The method of claim 34, wherein concentrations of said Group VIII B metal or compound thereof, said bromide source and said polyaniline are selected by said genetic algorithm screening process.

39. The method of claim 34, wherein said Group VIII B metal or compound thereof, said bromide source and said polyaniline are selected by said genetic algorithm screening process and concentrations thereof are selected by said algorithm screening process.

40. A method of selecting a carbonylation catalyst, comprising:

(A) synthesizing a first population of prospective carbonylation catalyst entities and detecting a property of each of said entities; and

(B) executing a genetic algorithm based on said property of said entities to identify a second population of prospective carbonylation catalyst entities.

41. A system for screening constructs to determine a problem solution, comprising:

a generator to provide a binary string representing a random first population of said constructs;

a combinatorial reactor to synthesize each construct according to said representation of said first population and to determine a fitness function for each construct of said population by a high throughput screening process; and

an executor to execute a genetic algorithm on said first population to produce a generation that defines a second population of said materials.